# Self-assembly of a new cobalt complex, (C6H14N2)3[CoCl4]Cl : Synthesis, empirical and DFT calculations

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**Table captions**

**Table S1:** Crystal data and structure parameters for (C6H14N)3[CoCl4]Cl.

**Table S2:** Enrichment ratio of different inter-contact and percentage of each atom on HS in (C6H14N)3[CoCl4]Cl.

**Table S3:** Global reactivity descriptors and calculated frontier molecular orbital parameters of (C6H14N)3[CoCl4]Cl compound.

**Figure captions**

**Fig. S1.** 2D-FP of the main interactions in the crystal packing and % age of atoms present in (C6H14N)3[CoCl4]Cl.

**Fig. S2.** Percentage of atoms present in (C6H14N)3[CoCl4]Cl.

**Fig. S3.** Theoretical and experimental IR spectrum of (C6H14N)3[CoCl4]Cl.

**Fig. S4.** DTA and TG curves of (C6H14N)3[CoCl4]Cl.

**Fig.S5.** HOMO-LUMO orbital plots of (C6H14N)3[CoCl4]Cl computed with B3LYP/6-311+G(d,p).

**Table S1:** Crystal data and structure parameters for (C6H14N)3[CoCl4]Cl.

CCDC 2102182

Temperature 150K

Empirical formula 3(C6H14N)·Cl4Co·Cl

Formula weight (g mol-1) 536.72

Crystal system Monoclinic

Space group *P*21/n

a 15.2645 (12) Å

b 10.0843(7) Å

c 17.4450(13) Å

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Z 4

V 2670.8 (3) Å3

F(000) 1132

µ(Mo Kα) 0.71073 Å

Index ranges −19<hmax<19, −13<kmax<13, −22<lmax<22

Reflections collected 24384

Independent reflections 6103

Reflections with I>2σ(I) 4718

Rint 0.037

Absorption correction: *multi-scan* Tmin= 0.703, Tmax = 0.813

Refined parameters 271

R[F2> 2σ(F2)] 0.032

w*R*(F2) 0.071

Goodness of fit 1.03

Δρmax= 0.63 e Å−3 Δρmin=-0.58e Å−3

**Table S2:** Enrichment ratio of different inter-contact and percentage of each atom on HS in (C6H14N)3[CoCl4]Cl.

|  |  |  |  |
| --- | --- | --- | --- |
| **RE** | **H** | **Co** | **Cl** |
| **H** | 0.95 | - | 1.24 |
| **Co** |  | - | - |
| **Cl** |  | - | - |
| **%surface** | 79.45 | 0.25 | 19.8 |

**Table S3:** Global reactivity descriptors and calculated frontier molecular orbital parameters of (C6H14N)3[CoCl4]Cl using DFT/LANL2DZ level.

|  |
| --- |
|  |
| **Parameters (eV)** |  |
| EHOMO |

|  |
| --- |
| -6.027913632 |

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| ELUMO | -3.459138592 |
| ∆E= ELUMO- EHOMO | **2.56877504** |
| EHOMO-1 | -6.276627656 |
| ELUMO+1 | 0.568178208 |
| ∆E= ELUMO+1- EHOMO-1 | **6.844805864** |
| Chemical potential (μ) | -4.743526112 |
| Softness (ς) | 0.389290609 |
| Ionization energy (I) | 6.027913632 |
| Electron affinity (A) | 3.459138592 |
| Electronegativity (χ) | 4.788526112 |
| Chemical hardness (η) | 1.28438752 |
| Electrophilicity index (ω) | 8.759443557 |



**Fig. S1**

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**Fig. S2.** Percentage of atoms present in (C6H14N)3[CoCl4]Cl.



**Fig. S3.** Theoretical and experimental IR spectrum of (C6H14N)3[CoCl4]Cl.



**Fig. S4**



**Fig. S5**